Texas A & M Univ. NsG-239-62

UNPUBLISHED PRELIMINARY DATA N65-16843

A MATHEMATICAL INVESTIGATION OF THE [redacted] STRUCTURE OF LIGHT METALS

4p (NASA Grant NsG-239-62)

(NASA CR-51664)

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I. Introduction

The availability of the Data Processing Center IBM 709 Computer and recent interest and advances in the art of numerical solutions of the Schrodinger's equations for atomic, molecular, and solid state physics suggested the problem of developing the computing capability of the Mathematics Department along the lines of numerical solutions of the equations of quantum mechanics.

A proposal to begin such a development received support from Research Grant No. NsG 239-62 in the spring of 1962, with actual funding to begin February, 1963. In an attempt to channel the efforts immediately into productive ground, a suggestion of W. Marshall, Division Leader, Theoretical Physics Division, Atomic Energy Research Establishment, Harwell, England was made the goal of the project. This suggestion was conveyed to us by J. L. Gammel, Head, Theoretical Nuclear Physics Group, Los Alamos Scientific Laboratories, Los Alamos, New Mexico. Dr. Marshall suggested in (2) and in private conversation with Dr. Gammel that a fruitful investigation of the electron nucleus interaction in many ions, starting first with neutral Li, might be made by means of the Unrestricted Hartree-Fock method.

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Neutral Li has 3 electrons, and its total spin is $S = 1/2$. According to the usual ideas, it is in a $(1s)^2$ $(2s)$ configuration. The electron nucleus interaction is proportional to $\sum s_i . I\rho_i$ where I is the spin of the nucleus, s_i is the spin of the ith electron, and where ρ_i is the density of the ith electron at the nucleus. The contributions due to the two electrons in the 1s orbital cancel because their spins are opposite, so one only needs

$$\rho \cong |\psi_{2s}(0)|^2$$

that is, the magnitude of the square of the wave function evaluated at the nucleus (that is, the origin).

The only trouble is--the answer is wrong. Marshall thinks one might improve the situation by taking the 1s states with spin up and spin down to be different. This amounts to considering the problem from the Unrestricted Hartree viewpoint rather than the Restricted.

II. Progress and Future Plans

It was decided in February, 1963 to begin with the Restricted Hartree-Fock procedures in the case of complete groups of electrons where the problem assumes its simplest form. Very fortunately, it now appears, we selected normal, atomic beryllium for our first problem. We began the organization of the problem in the spring of 1963 with the work progressing smoothly. Actual coding of the computer program was begun in April, 1963. The program was checked out for the calculation of atomic beryllium by the Hartree-Fock equations without exchange by the middle of June, 1963.

It was decided to write up a detailed preliminary progress report both on the Hartree-Fock procedures for beryllium and on the operating code.

This task was completed at the beginning of August, 1963 and the resulting report has been forwarded to the National Aeronautics and Space Administration under separated cover as Detailed Technical Supplement on Space Technology Project No. 5 (Hartree-Fock Solutions Without Exchange for Normal Beryllium). The coding of the program for the calculation of the Hartree-Fock equations with exchange was completed at the end of July, 1963. It is expected that this program will be in operation by the end of August, 1963.

The present opinion of the investigators is that the program for beryllium can be modified to run for lithium with minor changes. However, the emphasis on lithium has changed for two reasons. First, K. F. Berggren and R. F. Woods (1) have reached the conclusion that the usual interpretation of the results obtained for lithium by means of the Unrestricted Hartree-Fock equations are not entirely acceptable. Second, it appears that the investigations of atomic beryllium which are presently underway can be most usefully continued to the study of solid state or metallic beryllium

The Principal Investigator, Professor E. R. Keown of the Mathematics Department, has been invited to spend the year beginning September , 1963 with the Solid State and Molecular Theory Group of the Physics Department, Massachusetts Institute of Technology. This invitation is a direct outgrowth of the present investigation sponsored under Research Grant No. NsG 239-62. The research undertaken by Dr. Keown will be an extension of the Hartree-Fock results for atomic metals, beryllium in particular, to studies of the solid state metals by means of the Augmented Plane Wave Techniques of Prof. J. C. Slater of that Group.

III. References

(1) K. F. Berggren and R. F. Woods, Effect of Correlation on the Hyperfine Interaction in Lithium, Phys. Rev., 130(1963), pages 198-205.

(2) W. Marshall, The Unrestricted Hartree-Fock Method, Proc. Phys. Soc., Vol. LXXVII(1961), pages 113-119.